# Supplementary Information

*Vadim R. Ziatdinov,[†] Jonas I. Oxgaard,[‡] Oleg A. Mironov,[†] Kenneth J. H. Young,[†]*

*William A. Goddard[‡]* and Roy A. Periana*[†].*

University of Southern California, Department of Chemistry, Loker Hydrocarbon Institute, Los Angeles, California 90089

Materials and Process Simulation Center, Beckman Institute (139-74), Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125

E-mail: rperiana@usc.edu

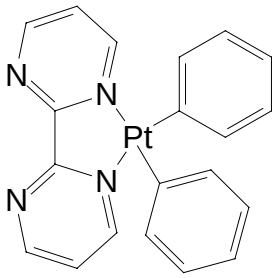
**General.** Unless otherwise noted, all reactions and manipulations were performed in a M-Braun circulating Argon atmosphere glovebox or using standard Schlenk techniques. Glassware was dried in an oven at 150 °C before use. Unless otherwise noted, reagents were purchased from commercial suppliers and used without further purification. Neutral alumina was used in chromatography unless otherwise noted. Diethyl ether, THF and benzene were distilled from sodium/benzophenone ketyl under Argon prior to use. Hexanes and pentane were dried with $P_2O_5$ under Argon and kept refluxing under flow of Argon. $CH_2Cl_2$ was purified from stabilizer by stirring with concentrated $H_2SO_4$ for 4 hours, mixture was separated, organic phase was neutralized with $KHCO_3$, dried with $MgSO_4$ and $P_2O_5$, and refluxed under flow of Argon for 3 days. Organic acids were distilled from $P_2O_5$. Deuterated solvents were degassed by freezing, evacuating, and thawing (3x), and were then dried over 4 Å sieves and stored under Argon.

Unless otherwise indicated, NMR spectra were obtained using a Variant Mercury-400 MHz

spectrometer (400 MHz for $_1$H spectra, 100.6 MHz for $^{13}C\{^1H\}$ spectra, 376.5 MHz for $^{19}F$ spectra). Chemical shifts are reported in parts per millio relative to residual protiated solvent, coupling constants are reported in Hertz (Hz), and integrations are reported in number of protons. Unless otherwise noted, samples for NMR analysis were prepared using $CDCl_3$ as the solvent.

Kinetic studies were performed using a Shimadzu-QP5000 GCMS or by NMR spectroscopy using a Variant Mercury-400 spectrometer (see above). All reaction mixtures were prepared under Argon and kept under static Ag during the kinetic analyses. For GCMS experiments, ethane standard was introduced.

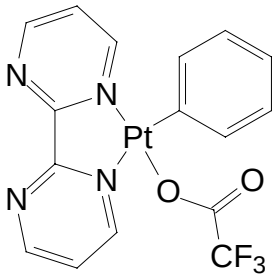
The compounds $[(Et_2S)Pt(Ph)_2]_2$[1], $K(pic)PtCl_2$[2] were prepared using literature procedures.



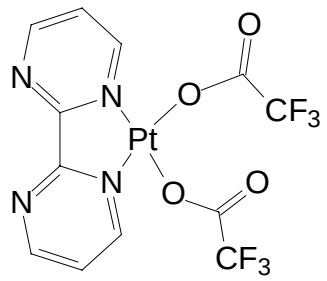

**(Bpym)Pt(Ph)$_2$. Method A**. In a 100 mL Schlenk flask containing 0.79 g (5.0 mmol, 400% excess) of bipymidine was added 20 mL of $CH_2Cl_2$ and vigorously stirred. In another 100 mL Schlenk flask containing 1.76 g (2.0 mmol) of $[(Et_2S)Pt(Ph)_2]_2$ was added in 80 mL of $CH_2Cl_2$ to complete solid dissolving and added drop-wise to the first flask. The solution color changed from slight yellow to deep red during reaction and black solid of bi-adduct to ligand precipitate. The volume was reduced to 50 mL and the solid was precipitated with methanol (200 mL) to leave excess of free ligand in solution. The solid was washed three times with methanol, dried in vacuo over 1 day and a red crystalline solid formed (1.6 g, 80% yield).

**Method B.** In a 100 mL Schlenk flask containing 0.79 g (5.0 mmol, 20% excess) of bipymidine was added 20 mL of $CH_2Cl_2$, cooled to $-50^oC$ and vigorously stirred. In another 100 mL Schlenk flask containing 1.76 g (2.0 mmol) of $[(Et_2S)Pt(Ph)_2]_2$ was added in 80 mL of $CH_2Cl_2$ to complete solid dissolving and added drop-wise to the first flask. The reaction mixture was allowed to warm up till room

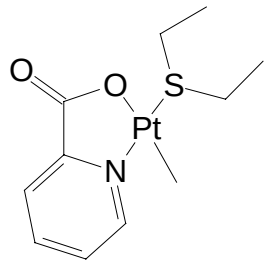
temperature for 5 hours. The solution color changed from slight yellow to deep red during reaction at 0°C. The volume was reduced to 30 mL and the solid was precipitated with methanol (100 mL) to leave excess of free ligand in solution. The solid was washed with methanol, dried in vacuo over 1 day and a red crystalline solid formed (1.8 g, 90% yield). $^{1}$H NMR (400 MHz, $CDCl_3$, 298 K): 9.20 (dd, 2H, H-6, $^{3}J$ = 4.9 Hz, $^{4}J$ = 2.2 Hz), 8.79 (dd, 2H, H-4, $^{3}J$ = 5.5 Hz, $^{4}J$ = 2.3 Hz), 7.50 (t, 2H, H-4, $^{3}J$ = 5.3 Hz), 7.38 (dd, 2H, H-orto, $^{3}J$ = 8.2 Hz, $^{4}J$ = 1.6 Hz, w/Pt satellites $^{3}J_{Pt-H}$ = 35 Hz), 7.00 (t, 2H, H-meta, $^{3}J$ = 7.4 Hz), 6.87 (tt, 1H, H-para, $^{3}J$ = 7.4 Hz, $^{4}J$ = 1.4 Hz). HRMS (Electro-spray) Calcd for $C_{20}H_{17}N_4Pt$ (M+H): 508.1101. Found: 508.1114.




**(Bpym)Pt(Ph)(TFA).** In a 100 mL Schlenk flask containing 202.8 mg (0.40 mmol) of (bpym)Pt(Ph)$_2$ was added in 50 mL of $CH_2Cl_2$ to complete dissolving, and added 32.0 μL (0.41 mmol, slight excess) of trifluoroacetic acid. The solution was allowed to react at room temperature for 2 hours. The volume was reduced to 10 mL and the solid was precipitated with methanol (50 mL) to leave trace of (bpym)Pt(TFA)$_2$ in solution. The solvent residue was dried in vacuo over 1 day and a red crystalline solid formed (207 mg, 95% yield). $^{1}$H NMR (400 MHz, $CD_2Cl_2$, 298 K): 9.77 (dd, 1H, H-6, $^{3}J$ = 5.4 Hz, $^{4}J$ = 2.2 Hz), 9.27 (dd, 1H, H-4, $^{3}J$ = 4.8 Hz, $^{4}J$ = 2.2 Hz), 9.24 (dd, 1H, H-4, $^{3}J$ = 4.8 Hz, $^{4}J$ = 2.2 Hz), 8.86 (dd, 1H, H-6, $^{3}J$ = 5.8 Hz, $^{4}J$ = 2.2 Hz, w/Pt satellites $^{3}J_{Pt-H}$ = 28.2 Hz), 7.84 (t, 1H, H-5, $^{3}J$ = 5.1 Hz), 7.46 (t, 1H, H-4, $^{3}J$ = 5.3 Hz), 7.35 (dd, 2H, H-orto, $^{3}J$ = 8.0 Hz, $^{4}J$ = 1.2 Hz, w/Pt satellites $^{3}J_{Pt-H}$ = 17.6 Hz), 7.09 (t, 2H, H-meta, $^{3}J$ = 7.4 Hz), 1.39 (tt, 1H, H-para, $^{3}J$ = 7.4 Hz, $^{4}J$ = 1.2 Hz). $^{13}$C NMR (101 MHz, $CDCl_3$, 298 K): 159.9 (s), 157.7 (s), 157.3 (s), 155.3 (s), 137.5 (s), 128.0 (s), 124.9 (s), 124.7 (s), 124.2 (s). $^{19}$F NMR (101 MHz, $CD_2Cl_2$, 298 K, with $C_6F_6$ as standard -164.9): -77.6 (s). Anal. Calcd for $C_{16}H_{11}N_4O_2PtF_3$: C, 35.37; H, 2.04; N, 10.31; F, 10.49. Found: C, 36.53; H, 1.93; N, 9.84; F, 10.06.

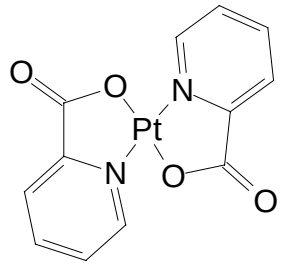


**(Bpym)Pt(TFA)$_2$.** In a 100 mL Schlenk flask containing 108.6 mg (0.20 mmol) of (bpym)Pt(Ph)$_2$ was completely dissolved in 50 mL of $CH_2Cl_2$ to complete dissolving, and added 24.0 μL (0.3 mmol, excess) of trifluoroacetic acid. The solution was allowed to react at room temperature for 2 hours. The solvent was dried in vacuo over 1 day and a yellow crystalline solid formed (115 mg, 100% yield). $^1$H NMR (400 MHz, $CD_2Cl_2$, 298 K): 9.32 (dd, 2H, H-6, $^3J$ = 5.0 Hz, $^4J$ = 1.9 Hz), 8.89 (dd, 2H, H-4, $^3J$ = 5.9 Hz, $^4J$ = 2.0 Hz), 7.84 (t, 2H, H-5, $^3J$ = 5.4 Hz). $^{13}$C NMR (101 MHz, acetone-d6, 298 K): 163.43 (s, -CO2-), 162.56 (s, pym), 161.57 (s, pym), 157.07 (s, pym), 125.58 (s, pym), 117.24 (s, -$CF_3$). $^{19}$F NMR (101 MHz, $CD_2Cl_2$, 298 K, with $C_6F_6$ as standard - -164.9): -75.26 (s, $CF_3$). Anal. Calcd for $C_{12}H_6N_4O_4PtF_6$: C, 25.07; H, 1.10; N, 9.32; F, 19.34. Found: C, 24.88; H, 1.04; N, 9.67; F, 19.68. MS (Electro-spray) Calcd for $C_{10}H_6O_2N_4F_3Pt$ (M-TFA): 466.0091. Found: 466.0092.

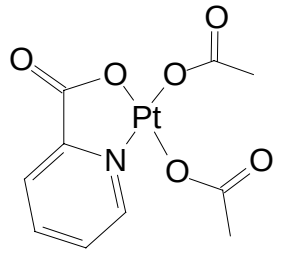


**(Pic)Pt(Me)(Et$_2$S).** In a 50 mL Schlenk flask containing 189.0 mg (0.3 mmol) of dimmer [(Et$_2$S)Pt(Me)$_2$]$_2$ was added 73.8 mg (0.6 mmol) of picolinic acid and $CHCl_3$ (20 mL). The solution was stirred and heated at 70$^o$C for 1 hour. The crystalline solid was precipitated with pentane (60 mL) and filtered. At this point NMR show small presence of Platinum starting material that was removed by column chromatography with pentane/EtOAc 1:1 mixture as solvent. The solvent has been removed in vacuo over 1 day and a white crystalline solid formed (240 mg, 91% yield). $^1$H NMR (400 MHz, $CDCl_3$, 298 K): 8.62 (d, 1H, H-6, $^3J$ = 5.6 Hz, w/Pt satellites $^3J_{Pt-H}$ = 24 Hz), 8.17 (dd, 1H, H-3, $^3J$ = 7.9 Hz, $^4J$ =

1.4 Hz), 8.05 (dt, 1H, H-4, $^{3}J$ = 7.8 Hz, $^{4}J$ = 1.3 Hz), 7.52 (ddd, 1H, H-5, $^{3'}J$ = 7.4 Hz, $^{3''}J$ = 5.8 Hz, $^{4}J$ = 1.6 Hz), 3.10 (bm, 2H, S-$CH_2$-Me), 2.85 (bm, 2H, S-$CH_2$-Me), 1.39 (t, 6H, S-$CH_2$-$CH_3$, $^{3}J$ = 7.5 Hz) and 0.73 (s, 3H, Pt-$CH_3$, w/Pt satellites, $^{2}J_{Pt-H}$ = 41.4 Hz). $^{13}$C NMR (101 MHz, $CDCl_3$, 298 K): 172.5 (s, -$CO_2$-), 153.5 (s, py), 144.64 (s, py), 139.2 (s, py), 128.3 (s, py), 127.5 (s, py), 30.7 (s, -$CH_2$-), 13.2 (s, -$CH_3$), and -22.2 (s, Pt-Me). Anal. Calcd for $C_{11}H_{17}NO_2PtS$: C, 31.28; H, 4.06; N, 3.32; S, 7.59. Found: C, 31.52; H, 3.81; N, 3.23; S, 7.86.




**$(Pic)_2Pt$.** In a 50 mL Schlenk flask containing 415.0 mg (1.0 mmol) of $K_2PtCl_4$ was added 246.2 mg (2.0 mmol) of picolinic acid and water (10 mL). The solution was stirred and heated at 70$^{o}$C for 5 minutes to dissolve all starting materials. The white precipitate was formed, filtered, washed with water, MeOH and dried in vacuum (420 mg, 96% yield). $^{1}$H NMR (400 MHz, trufluoroacetic acid-$d_1$, 298 K): 8.61 (d, 1H, H-6, $^{3}J$ = 5.7 Hz), 8.23 (t, 1H, H-4, $^{3}J$ = 8.3 Hz), 8.01 (d, 1H, H-3, $^{3}J$ = 7.9 Hz), 7.72 (t, 1H, H-5, $^{3}J$ = 6.6 Hz). $^{13}$C NMR (101 MHz, trufluoroacetic acid-$d_1$, 298 K): 182.01 (s, -CO2-), 150.76 (d, py), 143.79 (s, py), 132.27 (s, py), 130.20 (s, py). Anal. Calcd for $C_{12}H_8N_2O_4Pt$: C, 32.75; H, 1.96; N, 6.22. Found: C, 32.81; H, 1.84; N, 6.38.




**K(Pic)Pt(OAc)$_2$ in solution.** In a 15 mL Schlenk flask containing 42.7 mg (0.1 mmol) of $KpicPtCl_2$ was added 33.4 mg (0.2 mmol) of silver acetate and TFA (5 mL). The solution was stirred and heated at

70°C for 5 minutes to dissolve all starting materials. The white precipitate of AgCl was formed, filtered out and the solution was analyzed. $^{1}$H NMR (400 MHz, trufluoroacetic acid-$d_1$, 298 K): 8.78 (s, 1H), 8.72 (s, 1H), 8.51 (s, 1H), 8.20 (s, 1H), 2.70 (s, 6H). $^{13}$C NMR (101 MHz, trufluoroacetic acid-$d_1$, 298 K): 183.10 (s, -OC(O)py), 180.72 (s, -OC(O)Me), 149.94 (d, py), 143.79 (s, py), 131.82 (s, py), 130.52 (s, py), 20.58 (s, -$CH_3$), 20.40 (s, -$CH_3$). HRMS (Electro-spray) Calcd for $C_{10}H_{10}NO_6Pt$ (M-K): 435.0156. Found: 435.0156.

**Stability study.** In a NMR tube containing 1mg (2 μmol) of (pic)$PtCl_2$, 0.5mg (0.02 μmol) of silver acetate was added 1mL of TFA-d1. The mixture was heated at 100°C and analyzed by NMR.

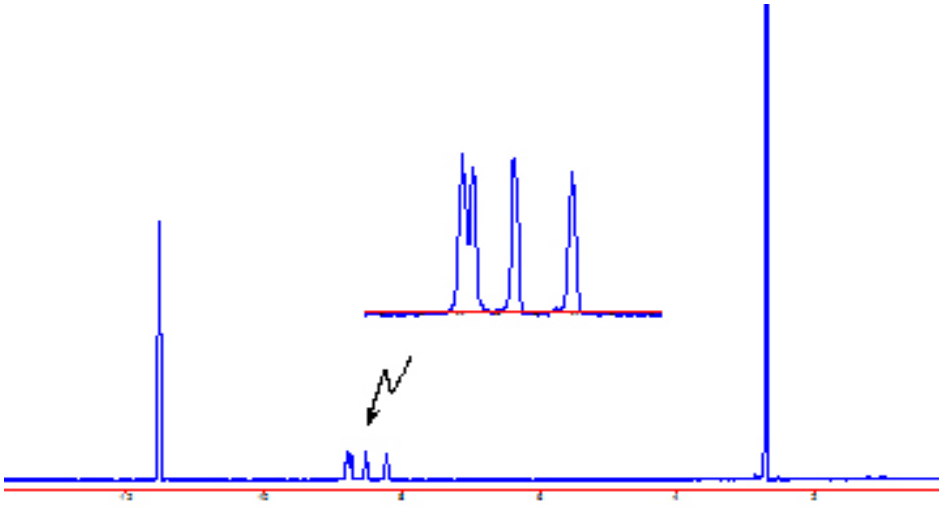


**Figure 1**. $^{1}$H NMR of Platinum picolinate in trifluoroacetic acid after one day at 100°C

**Deuterium insertion study.** In a 3 mL Schlenk flask containing 1mg (2 μmol) of (pic)PtCl2, 0.5mg (2 μmol) of silver acetate was added 1mL of TFA-d1 and 0.1 mL of benzene. The mixture was let to react and AgCl was removed by filtration. The mixture was heated at 70°C, cooled down to room temperature and 1 μL of reaction solution was injected to GC/MS. After separation on column and ionization the mass distribution of ions of injected sample was collected. The deconvolution program converts the mass distribution of ion to benzene isotope concentration. This program used experimental data of different isotopes of benzene to construct the system of linear equations, by solving which the isotope distribution of benzene in sample was determined. According to test experiments this approach can be

reliable to within 2%." The same procedure was used for 150°C.

| isotop\time | 0 | 20 | 40 | 60 | 80 | 100 | minutes |
|---|---|---|---|---|---|---|---|
| TOF | start | 0.0155 | 0.0127 | 0.0120 | 0.0102 | 0.0093 | |
| TON | | 18.6 | 30.5 | 43.3 | 49.0 | 55.9 | |
| d0 | 99.4 | 96.7 | 94.3 | 91.4 | 89.7 | 88.0 | |
| d1 | 0.1 | 2.3 | 3.6 | 5.6 | 6.8 | 8.1 | |
| d2 | 0.1 | 0.1 | 0.5 | 0.8 | 1.0 | 1.2 | |
| d3 | 0.0 | 0.1 | 0.3 | 0.5 | 0.6 | 0.7 | |
| d4 | 0.0 | 0.0 | 0.3 | 0.5 | 0.6 | 0.7 | |
| d5 | 0.0 | 0.1 | 0.3 | 0.5 | 0.6 | 0.7 | |
| d6 | 0.4 | 0.7 | 0.7 | 0.7 | 0.5 | 0.6 | |

**Deuterium insertion study.** In a 3 mL Schlenk flask containing 1mg (2 μmol) of (bpym)Pt(TFA)$_2$, 0.5mg (2 μmol) of silver acetate was added 1mL of TFA-d1 and 0.1 mL of benzene. The mixture was heated at 70°C and analyzed by GC/MS as above.

| isotop\time | 0 | 20 min | 43 min | 63 min | 20 h | 42 h | 60 hours |
|---|---|---|---|---|---|---|---|
| TOF | 0 | 0 | 0 | 0 | 6.37298E-05 | 6.19043E-05 | 5.60209E-05 |
| TON | 0.0 | 0.0 | 0.0 | 0.0 | 4.6 | 9.4 | 12.1 |
| D0 | 99.6 | 99.9 | 99.3 | 99.6 | 98.8 | 97.4 | 96.8 |
| D1 | 0.4 | 0.1 | 0.7 | 0.4 | 0.8 | 1.8 | 2.1 |
| D2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 0.5 | 0.8 |
| D3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.2 | 0.3 |
| D4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.1 | 0.1 |
| D5 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| D6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

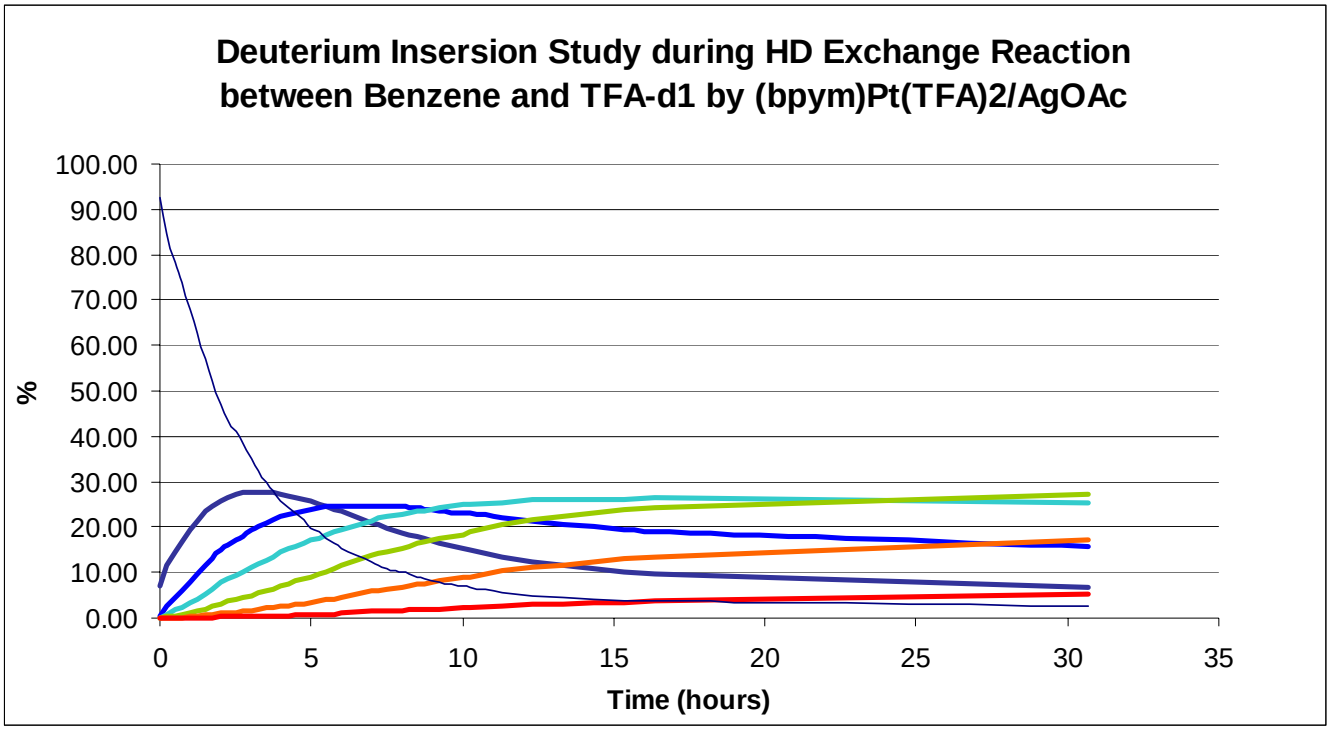
**Deuterium insertion study.** In a 3 mL Schlenk flask containing 1mL of TFA-d1 and 0.1 mL of benzene and 0.5mg (2 μmol) of silver acetate was heated at 70°C and analyzed by GC/MS as above.

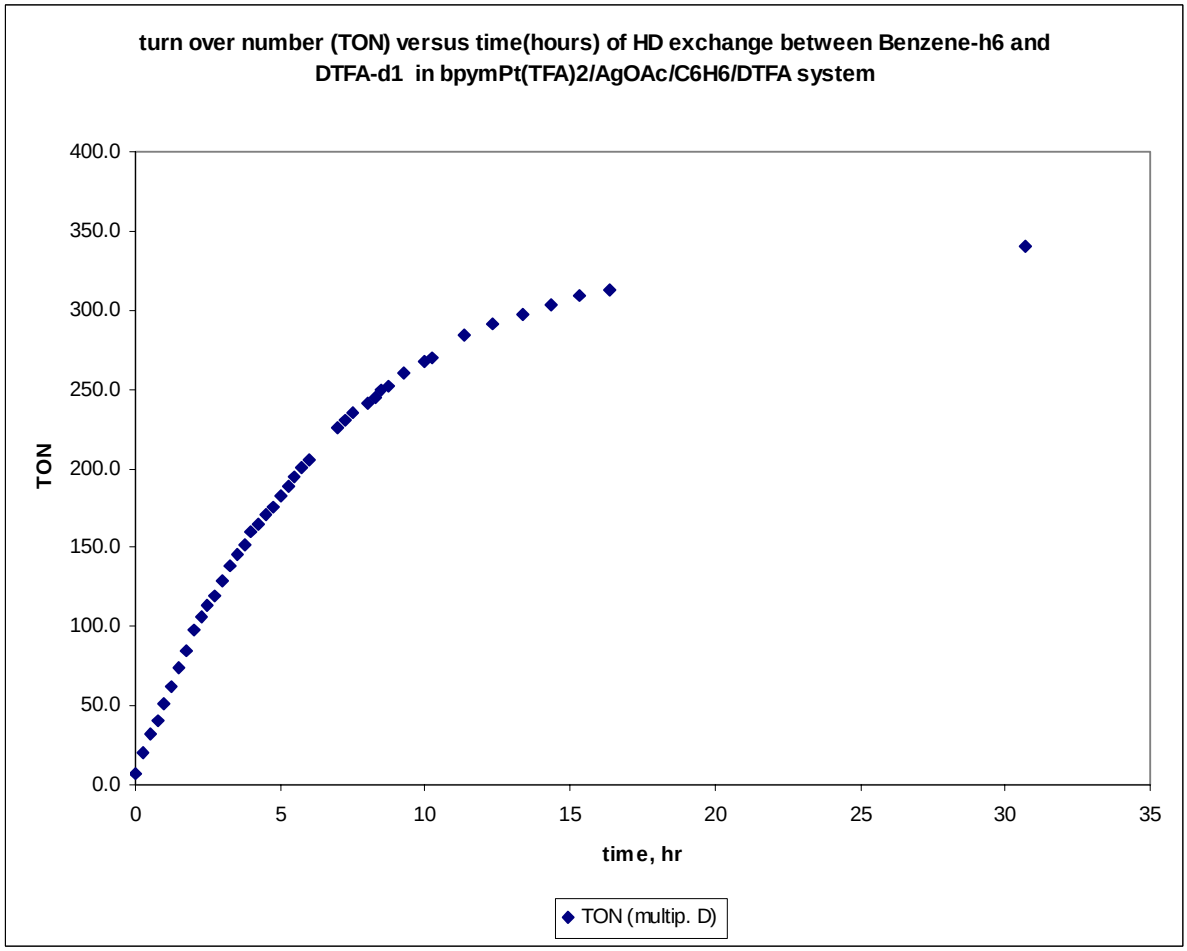
| isotop\time | 0 | 20 min | 43 min | 63 min | 20 hours | 42 hours | 60 hours |
|---|---|---|---|---|---|---|---|
| TOF | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| TON | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| d0 | 100.0 | 99.8 | 99.5 | 99.7 | 99.3 | 99.3 | 99.9 |
| d1 | 0.0 | 0.2 | 0.5 | 0.3 | 0.7 | 0.7 | 0.1 |
| d2 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| d3 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| D4 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| D5 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| D6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

**Deuterium insertion study.** In a 3 mL Schlenk flask containing 5mg (0.01 mmol) of

(bpym)Pt(TFA)$_2$, 3mg (0.02 mmol) of silver acetate was added 1mL of TFA-d1 and 0.1 mL of benzene. The mixture was heated at 150$^o$C analyzed by GC/MS every 15 minutes as above.

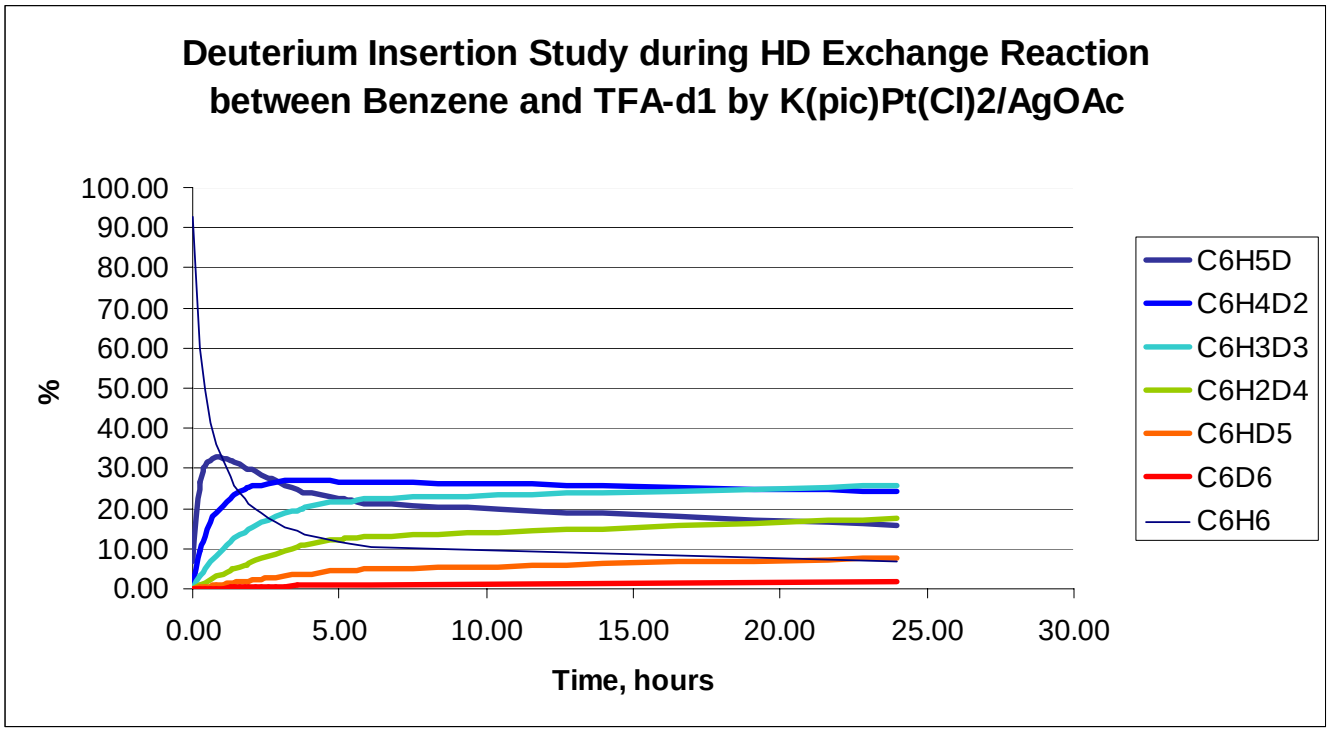
| t (hr) | d0 | d1 | d2 | d3 | d4 | d5 | d6 | t (min) | TON |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 92.51 | 7.26 | 0.22 | 0.01 | 0.00 | 0.00 | 0.00 | 0 | 7.7 |
| 0.25 | 84.80 | 11.44 | 2.58 | 0.88 | 0.25 | 0.05 | 0.01 | 15 | 20.5 |
| 0.5 | 78.28 | 14.66 | 4.64 | 1.73 | 0.55 | 0.12 | 0.02 | 30 | 32.1 |
| 0.75 | 73.87 | 16.79 | 6.02 | 2.34 | 0.77 | 0.18 | 0.03 | 45 | 40.0 |
| 1 | 67.98 | 19.39 | 7.93 | 3.23 | 1.12 | 0.29 | 0.05 | 60 | 51.2 |
| 1.25 | 62.73 | 21.41 | 9.70 | 4.17 | 1.51 | 0.41 | 0.07 | 75 | 61.8 |
| 1.5 | 56.94 | 23.38 | 11.61 | 5.33 | 2.05 | 0.59 | 0.11 | 90 | 74.4 |
| 1.75 | 52.36 | 24.77 | 13.21 | 6.30 | 2.48 | 0.73 | 0.14 | 105 | 84.5 |
| 2 | 47.09 | 25.88 | 15.06 | 7.65 | 3.16 | 0.97 | 0.19 | 120 | 97.6 |
| 2.25 | 43.67 | 26.56 | 16.22 | 8.53 | 3.65 | 1.15 | 0.22 | 135 | 106.2 |
| 2.5 | 40.89 | 27.24 | 17.17 | 9.20 | 3.97 | 1.28 | 0.26 | 150 | 113.0 |
| 2.75 | 38.56 | 27.44 | 18.06 | 9.92 | 4.36 | 1.39 | 0.28 | 165 | 119.4 |
| 3 | 35.08 | 27.75 | 19.34 | 11.02 | 4.96 | 1.57 | 0.28 | 180 | 128.8 |
| 3.25 | 32.28 | 27.69 | 20.18 | 11.97 | 5.61 | 1.88 | 0.39 | 195 | 138.1 |
| 3.5 | 29.99 | 27.58 | 20.96 | 12.84 | 6.11 | 2.08 | 0.43 | 210 | 145.4 |
| 3.75 | 27.92 | 27.56 | 21.78 | 13.58 | 6.53 | 2.20 | 0.43 | 225 | 151.6 |
| 4 | 25.89 | 27.12 | 22.36 | 14.43 | 7.18 | 2.51 | 0.52 | 240 | 159.5 |
| 4.25 | 24.22 | 26.96 | 22.81 | 15.11 | 7.63 | 2.71 | 0.56 | 255 | 165.3 |
| 4.5 | 23.00 | 26.46 | 23.30 | 15.72 | 8.03 | 2.89 | 0.60 | 270 | 170.4 |
| 4.75 | 21.75 | 26.17 | 23.60 | 16.25 | 8.49 | 3.08 | 0.66 | 285 | 175.4 |
| 5 | 19.93 | 25.64 | 24.07 | 17.12 | 9.13 | 3.39 | 0.72 | 300 | 182.9 |
| 5.25 | 18.89 | 25.09 | 24.29 | 17.68 | 9.63 | 3.64 | 0.78 | 315 | 188.1 |
| 5.5 | 17.46 | 24.46 | 24.61 | 18.44 | 10.24 | 3.93 | 0.85 | 330 | 194.7 |
| 5.75 | 16.43 | 23.91 | 24.70 | 19.02 | 10.83 | 4.18 | 0.92 | 345 | 200.1 |
| 6 | 15.44 | 23.37 | 24.81 | 19.55 | 11.39 | 4.45 | 1.00 | 360 | 205.4 |
| 7 | 12.26 | 20.7725 | 24.7507 | 21.4014 | 13.6414 | 5.82214 | 1.35195 | 420 | 226.3 |
| 7.25 | 11.56 | 20.3807 | 24.7176 | 21.8355 | 14.0898 | 6.0365 | 1.37994 | 435 | 230.1 |
| 7.5 | 10.93 | 19.7355 | 24.5846 | 22.3436 | 14.5768 | 6.32334 | 1.50613 | 450 | 234.9 |
| 8 | 10.03 | 18.8349 | 24.592 | 22.8615 | 15.2796 | 6.78569 | 1.61634 | 480 | 241.3 |
| 8.25 | 9.62 | 18.3547 | 24.3998 | 23.1437 | 15.741 | 7.04868 | 1.69207 | 495 | 244.9 |
| 8.5 | 9.06 | 17.8362 | 24.1992 | 23.4539 | 16.2627 | 7.39826 | 1.78974 | 510 | 249.4 |
| 8.75 | 8.75 | 17.4817 | 23.9725 | 23.6808 | 16.6868 | 7.57758 | 1.85064 | 525 | 252.2 |
| 9.25 | 7.87 | 16.428 | 23.643 | 24.402 | 17.5006 | 8.15036 | 2.00597 | 555 | 259.7 |
| 10 | 7.06 | 15.4021 | 23.2497 | 24.8398 | 18.4473 | 8.8021 | 2.19899 | 600 | 267.4 |
| 10.25 | 6.84 | 15.0272 | 23.1552 | 24.9246 | 18.8494 | 8.96254 | 2.24101 | 615 | 269.8 |
| 11.333 | 5.68 | 13.2463 | 22.0149 | 25.5261 | 20.4758 | 10.3654 | 2.69135 | 680 | 283.7 |
| 12.333 | 5.03 | 12.2461 | 21.4065 | 25.9414 | 21.477 | 11.0395 | 2.85945 | 740 | 291.1 |
| 13.333 | 4.57 | 11.391 | 20.6912 | 26.222 | 22.3454 | 11.7015 | 3.07886 | 800 | 297.8 |
| 14.333 | 4.22 | 10.6726 | 20.0627 | 26.2457 | 23.1225 | 12.3919 | 3.28457 | 860 | 303.7 |
| 15.333 | 3.9 | 10.002 | 19.4384 | 26.3036 | 23.7809 | 13.0774 | 3.49764 | 920 | 309.3 |
| 16.333 | 3.64 | 9.525 | 19.0578 | 26.349 | 24.339 | 13.4659 | 3.62329 | 980 | 313.1 |
| 30.667 | 2.66305 | 6.74812 | 15.6241 | 25.4147 | 27.2668 | 17.0575 | 5.22578 | 1840 | 339.9 |

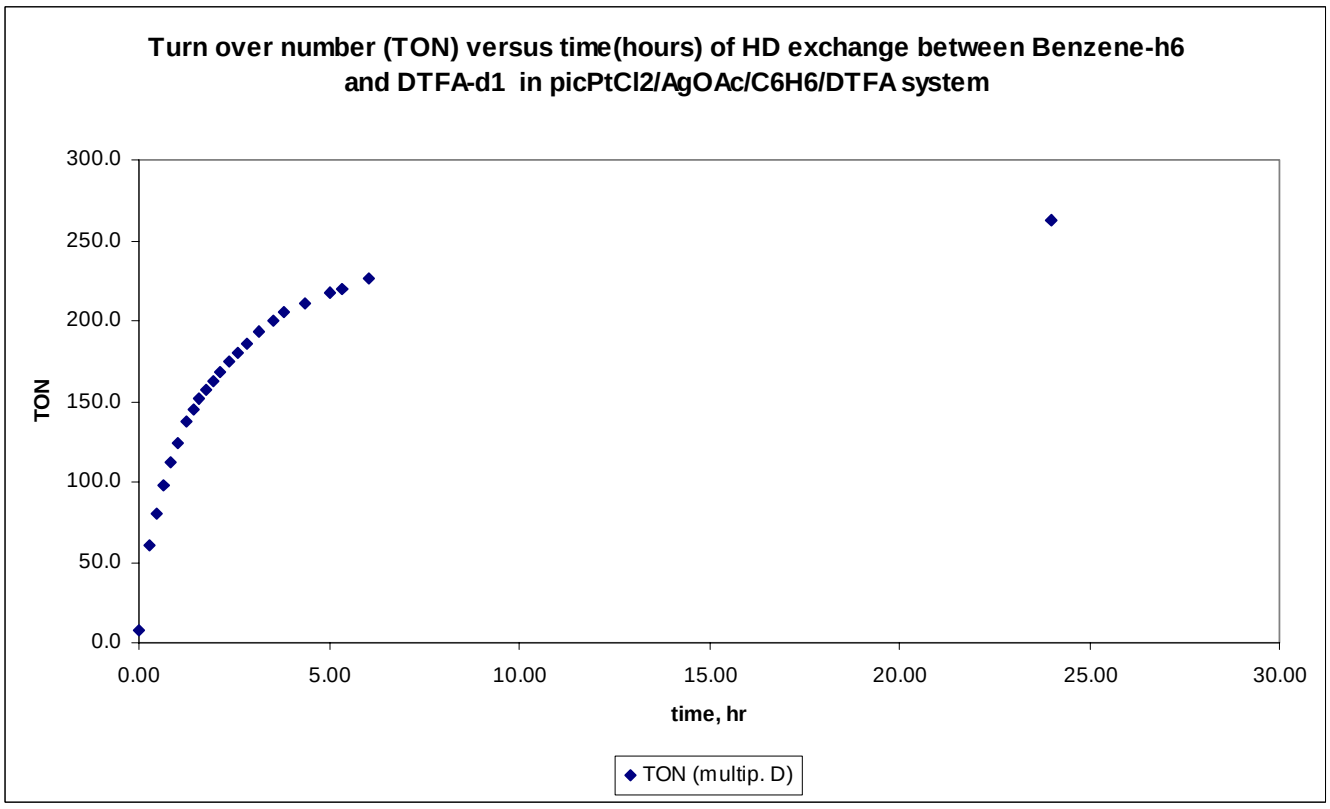

Deuterium Insersion Study during HD Exchange Reaction between Benzene and TFA-d1 by (bpym)Pt(TFA)2/AgOAc
100.00
90.00
80.00
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
%
0
5
10
15
20
25
30
35
Time (hours)


turn over number (TON) versus time(hours) of HD exchange between Benzene-h6 and DTFA-d1 in bpymPt(TFA)2/AgOAc/C6H6/DTFA system
400.0
350.0
300.0
250.0
200.0
150.0
100.0
50.0
0.0
TON
0
5
10
15
20
25
30
35
time, hr
TON (multip. D)

**Deuterium insertion study.** In a 3 mL Schlenk flask containing 5mg (0.01 mmol) of (pic)$Pt(Cl)_2$, 3mg (0.02 mmol) of silver acetate was added 1mL of TFA-d1 and 0.1 mL of benzene. Mixture was heated at 100$^{o}$C and analyzed by GC/MS every 15 minutes as above.

| time (hr) | d0 | d1 | d2 | d3 | d4 | d5 | d6 | TON |
|---|---|---|---|---|---|---|---|---|
| 0.00 | 92.99 | 6.76 | 0.22 | 0.02 | 0.01 | 0.00 | 0.00 | 7.3 |
| 0.27 | 59.79 | 26.54 | 9.32 | 3.06 | 0.98 | 0.26 | 0.05 | 59.9 |
| 0.45 | 49.41 | 30.54 | 13.19 | 4.82 | 1.56 | 0.41 | 0.08 | 80.1 |
| 0.63 | 41.54 | 32.20 | 16.56 | 6.70 | 2.29 | 0.60 | 0.10 | 98.2 |
| 0.82 | 36.24 | 32.78 | 18.87 | 8.25 | 2.94 | 0.79 | 0.14 | 111.8 |
| 1.02 | 31.95 | 32.55 | 20.75 | 9.87 | 3.69 | 1.02 | 0.17 | 124.5 |
| 1.27 | 28.02 | 31.87 | 22.56 | 11.53 | 4.51 | 1.28 | 0.23 | 137.4 |
| 1.43 | 25.74 | 31.41 | 23.52 | 12.53 | 5.07 | 1.47 | 0.26 | 145.2 |
| 1.60 | 24.09 | 30.88 | 24.19 | 13.35 | 5.57 | 1.63 | 0.29 | 151.5 |
| 1.77 | 22.64 | 30.27 | 24.73 | 14.15 | 6.06 | 1.82 | 0.33 | 157.5 |
| 1.93 | 21.30 | 29.76 | 25.12 | 14.94 | 6.51 | 2.01 | 0.36 | 163.1 |
| 2.13 | 19.99 | 29.12 | 25.63 | 15.68 | 7.05 | 2.16 | 0.37 | 168.6 |
| 2.35 | 18.80 | 28.37 | 25.86 | 16.53 | 7.62 | 2.39 | 0.43 | 174.7 |
| 2.60 | 17.67 | 27.67 | 26.23 | 17.21 | 8.14 | 2.60 | 0.47 | 180.2 |
| 2.83 | 16.66 | 26.94 | 26.46 | 17.93 | 8.68 | 2.83 | 0.50 | 185.5 |
| 3.15 | 15.40 | 25.64 | 26.82 | 18.78 | 9.53 | 3.20 | 0.62 | 193.5 |
| 3.55 | 14.26 | 24.68 | 26.92 | 19.56 | 10.26 | 3.62 | 0.70 | 200.5 |
| 3.82 | 13.33 | 24.03 | 27.11 | 20.14 | 10.83 | 3.81 | 0.75 | 205.6 |
| 4.38 | 12.44 | 23.30 | 26.81 | 21.00 | 11.50 | 4.15 | 0.80 | 211.5 |
| 5.00 | 11.60 | 22.31 | 26.72 | 21.63 | 12.26 | 4.57 | 0.91 | 218.0 |
| 5.33 | 11.44 | 22.10 | 26.55 | 21.77 | 12.52 | 4.69 | 0.93 | 219.6 |
| 6.07 | 10.56 | 21.19 | 26.50 | 22.44 | 13.21 | 5.06 | 1.05 | 225.9 |
| 24.00 | 6.71 | 15.82 | 24.49 | 25.57 | 17.78 | 7.83 | 1.80 | 262.6 |


Deuterium Insertion Study during HD Exchange Reaction between Benzene and TFA-d1 by K(pic)Pt(Cl)2/AgOAc
100.00
90.00
80.00
70.00
60.00
50.00
40.00
30.00
20.00
10.00
0.00
%
0.00
5.00
10.00
15.00
20.00
25.00
30.00
Time, hours
C6H5D
C6H4D2
C6H3D3
C6H2D4
C6HD5
C6D6
C6H6


Turn over number (TON) versus time(hours) of HD exchange between Benzene-h6 and DTFA-d1 in picPtCl2/AgOAc/C6H6/DTFA system
300.0
250.0
200.0
150.0
100.0
50.0
0.0
TON
0.00
5.00
10.00
15.00
20.00
25.00
30.00
time, hr
TON (multip. D)

Computational information:

bpym.Pt.TFA.TFA
Gas phase Energy: -1699.06522961581 hartrees
Solvation Energy: -1699.10667693293 hartrees
Zero Point Energy: 122.345 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Pt1 | -0.0001930497 | 0.0006646731 | -0.3502959436 |
| O2 | 1.5656885409 | -0.1440188960 | 0.9263090704 |
| C3 | 1.5422386601 | -0.8814676322 | 2.0056223061 |
| C4 | 2.9357494327 | -0.8304326925 | 2.6857233437 |
| F5 | 3.2335332964 | 0.4076939685 | 3.1157198312 |
| F6 | 3.9004971134 | -1.1949872070 | 1.7971020563 |
| F7 | 3.0062963939 | -1.6667823967 | 3.7249925917 |
| O8 | 0.6453514330 | -1.5549277511 | 2.4632610308 |
| N9 | 1.2966215441 | -0.1854104877 | -1.8967437911 |
| C10 | 2.7293794474 | -0.3899873835 | -4.1761489409 |
| C11 | 0.7357585082 | -0.1029112562 | -3.1344197769 |
| C12 | 2.6238948945 | -0.3772372149 | -1.7965351001 |
| C13 | 3.3896920660 | -0.4862194310 | -2.9502395998 |
| N14 | 1.4077565484 | -0.1992424186 | -4.2707647460 |
| H15 | 3.0119112775 | -0.4395437620 | -0.7836202643 |
| H16 | 4.4604451755 | -0.6423242691 | -2.8900502146 |
| H17 | 3.2721426693 | -0.4688047499 | -5.1147612150 |
| N18 | -1.2967126304 | 0.1889536931 | -1.8961645753 |
| C19 | -2.7298531546 | 0.3972882193 | -4.1747283242 |
| C20 | -0.7359714219 | 0.1089290042 | -3.1340682747 |
| C21 | -2.6238880413 | 0.3801539382 | -1.7952399800 |
| C22 | -3.3899248046 | 0.4909400549 | -2.9484203389 |
| N23 | -1.4081880288 | 0.2072090375 | -4.2700874206 |
| H24 | -3.0118024751 | 0.4404053369 | -0.7822887902 |
| H25 | -4.4607176619 | 0.6464184649 | -2.8876839806 |
| H26 | -3.2727808177 | 0.4776144251 | -5.1131018019 |
| O27 | -1.5661007747 | 0.1419659356 | 0.9267347079 |
| C28 | -1.5456126383 | 0.8892152631 | 1.9985458705 |
| O29 | -0.6528070816 | 1.5749807714 | 2.4463075893 |
| C30 | -2.9362789801 | 0.8323867615 | 2.6844422323 |
| F31 | -3.2246936578 | -0.4061007221 | 3.1182018401 |
| F32 | -3.9061093534 | 1.1897797357 | 1.7984428841 |
| F33 | -3.0084254756 | 1.6706533459 | 3.7225882235 |

bpym.Pt.TFA.C6H6+
Gas phase Energy: -1404.90071027875 hartrees
Solvation Energy: -1404.97776156501 hartrees
Zero Point Energy: 168.603 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Pt1 | -8.3752566511 | -3.5913463051 | 1.8076362701 |
| O2 | -7.7279478402 | -3.8821609140 | 3.7067966765 |
| C3 | -8.6378098305 | -3.7259138957 | 4.6398371054 |
| C4 | -8.0606406028 | -4.1184989253 | 6.0219709015 |
| F5 | -6.9414208449 | -3.4246197829 | 6.2946841354 |
| F6 | -7.7470757207 | -5.4367405067 | 6.0082830310 |
| F7 | -8.9452488059 | -3.9042105251 | 6.9920936923 |
| O8 | -9.7930351983 | -3.3752797356 | 4.5078451888 |
| N9 | -9.1198227050 | -3.6037294648 | -0.1289680283 |
| C10 | -10.3195938418 | -4.0045690043 | -2.5402473741 |
| C11 | -9.7501529236 | -4.7634749432 | -0.4745333127 |
| C12 | -9.0975347707 | -2.6181618850 | -1.0467748800 |
| C13 | -9.6955116703 | -2.7819848798 | -2.2882500545 |
| N14 | -10.3414996481 | -4.9874614444 | -1.6347045644 |
| H15 | -8.5959639875 | -1.6978620052 | -0.7735121676 |

| | | | |
|---|---|---|---|
| H16 | -9.6739451477 | -1.9855589601 | -3.0229443897 |
| H17 | -10.8133519323 | -4.2059234391 | -3.4872648232 |
| N18 | -9.0969443785 | -5.5088535834 | 1.7096438338 |
| C19 | -10.2228634853 | -7.9284446324 | 1.2734333345 |
| C20 | -9.7340878400 | -5.8323110903 | 0.5557995742 |
| C21 | -8.9972921862 | -6.4428206723 | 2.6744348479 |
| C22 | -9.5657194599 | -7.6956226625 | 2.4829196533 |
| N23 | -10.2976359720 | -7.0012891625 | 0.3105385700 |
| H24 | -8.4600547735 | -6.1628430704 | 3.5728192953 |
| H25 | -9.4970464574 | -8.4557632108 | 3.2525122937 |
| H26 | -10.6991753986 | -8.8824410354 | 1.0629439904 |
| H27 | -8.9197990079 | -0.9686370210 | 1.2971240961 |
| C28 | -8.1181232480 | -1.2409914048 | 1.9771193194 |
| C29 | -5.8700796742 | -1.3601235726 | 3.6558068390 |
| C30 | -8.2039783851 | -0.7835133765 | 3.3214309941 |
| C31 | -6.8765939613 | -1.7429938078 | 1.4876417873 |
| C32 | -5.7559102952 | -1.8041208334 | 2.3528599302 |
| C33 | -7.0939239695 | -0.8426820856 | 4.1392636598 |
| H34 | -9.1422766306 | -0.3796489982 | 3.6854493857 |
| H35 | -6.7144847965 | -1.8925073671 | 0.4244307700 |
| H36 | -4.8094240494 | -2.1758033889 | 1.9749213791 |
| H37 | -7.1547642896 | -0.4853338490 | 5.1625573805 |
| H38 | -5.0091781575 | -1.3948059245 | 4.3161492568 |

ts_bpym.Pt.Ph-H-TFA+
Gas phase Energy: -1404.88927933728 hartrees
Solvation Energy: -1404.95724370283 hartrees
Zero Point Energy: 165.507 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Pt1 | -6.4268866452 | -3.2154594379 | 1.8606988540 |
| O2 | -6.3300330917 | -5.1415022652 | 2.5572014327 |
| C3 | -6.3042747996 | -5.4676067588 | 3.7912180502 |
| C4 | -6.1913892938 | -6.9905092401 | 4.0491316020 |
| F5 | -4.8904831084 | -7.3157473631 | 4.1041854024 |
| F6 | -6.7649578963 | -7.6799965893 | 3.0521224651 |
| F7 | -6.7748486872 | -7.3168576219 | 5.1994399897 |
| O8 | -6.3183501762 | -4.6988209508 | 4.7677202741 |
| N9 | -6.5274972976 | -1.4715415975 | 0.7852959984 |
| C10 | -6.6721362260 | 0.5982999183 | -0.9784940540 |
| C11 | -6.5939018394 | -1.6373161448 | -0.5698178225 |
| C12 | -6.5327173665 | -0.2085808009 | 1.2550705324 |
| C13 | -6.6056855513 | 0.8726969149 | 0.3865571382 |
| N14 | -6.6649472612 | -0.6536168535 | -1.4480192218 |
| H15 | -6.4790135974 | -0.0845528932 | 2.3276781134 |
| H16 | -6.6104158246 | 1.8871545293 | 0.7679916055 |
| H17 | -6.7323698384 | 1.3929699343 | -1.7176825042 |
| N18 | -6.5129481264 | -3.9784391157 | -0.0756090758 |
| C19 | -6.6318927069 | -4.5960381989 | -2.7024279909 |
| C20 | -6.5839226006 | -3.0434690727 | -1.0515251663 |
| C21 | -6.5044350854 | -5.2763640699 | -0.4245467669 |
| C22 | -6.5638952412 | -5.6306395318 | -1.7667726544 |
| N23 | -6.6432360843 | -3.3053621251 | -2.3465618046 |
| H24 | -6.4516423962 | -5.9926623856 | 0.3886240518 |
| H25 | -6.5573291247 | -6.6721228986 | -2.0666093061 |
| H26 | -6.6795423298 | -4.8024766101 | -3.7685147231 |
| H27 | -4.1799491608 | -2.0801635857 | 3.8208405137 |
| C28 | -5.1121380310 | -1.6088688490 | 4.1204751287 |
| C29 | -7.5136405424 | -0.4382191324 | 4.9768035161 |
| C30 | -5.0795952485 | -0.4284715529 | 4.8542271350 |
| C31 | -6.3463001143 | -2.2369250752 | 3.7819373738 |
| C32 | -7.5455476764 | -1.6169815505 | 4.2402542560 |

| | | | |
|---|---|---|---|
| C33 | -6.2807172433 | 0.1568290342 | 5.2764838803 |
| H34 | -4.1310392534 | 0.0316191653 | 5.1138441701 |
| H35 | -8.4990371658 | -2.0962537952 | 4.0345950215 |
| H36 | -6.2550403708 | 1.0729684567 | 5.8604155643 |
| H37 | -8.4349632803 | 0.0134024876 | 5.3319917207 |
| H38 | -6.3345096021 | -3.4171815078 | 4.2404389392 |

bpym.Pt.TFA.Ph
grep: bpym.Pt.TFA.Ph.tfasolv.out: No such file or directory
Gas phase Energy: -1404.51995530512 hartrees
Zero Point Energy: 160.759 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Pt1 | -6.6211582892 | -2.0083261542 | 0.8294262878 |
| O2 | -6.1640323516 | -3.9954448115 | 0.7676290498 |
| C3 | -7.1215698399 | -4.8775548260 | 0.7942872469 |
| C4 | -6.5454244344 | -6.2807340281 | 0.4735664136 |
| F5 | -5.4785469635 | -6.5885316629 | 1.2323345418 |
| F6 | -6.1404378549 | -6.3060736571 | -0.8287388371 |
| F7 | -7.4605708757 | -7.2431055624 | 0.6292287974 |
| O8 | -8.3173708496 | -4.7318163345 | 0.9561447673 |
| N9 | -6.9113052650 | -0.0001264001 | 0.5755071900 |
| C10 | -7.2675418316 | 2.6175657867 | -0.0838490552 |
| C11 | -6.9939764046 | 0.4482779654 | -0.7135096382 |
| C12 | -6.9919012188 | 0.9202704852 | 1.5567526559 |
| C13 | -7.1733132056 | 2.2638979652 | 1.2603966306 |
| N14 | -7.1739947398 | 1.7140369882 | -1.0637718247 |
| H15 | -6.9204026811 | 0.5400455890 | 2.5690037155 |
| H16 | -7.2383521169 | 2.9998824280 | 2.0536153454 |
| H17 | -7.4168299654 | 3.6502777047 | -0.3899799453 |
| N18 | -6.5710124221 | -1.8262514492 | -1.3248676332 |
| C19 | -6.7970915830 | -1.2205979057 | -3.9482427407 |
| C20 | -6.8405810987 | -0.5830105101 | -1.7758142294 |
| C21 | -6.4002915848 | -2.8077594377 | -2.2223335807 |
| C22 | -6.5090844768 | -2.5366421497 | -3.5811234804 |
| N23 | -6.9604800154 | -0.2395300875 | -3.0542676876 |
| H24 | -6.1847904876 | -3.7929716640 | -1.8187272772 |
| H25 | -6.3790655759 | -3.3188947541 | -4.3201434671 |
| H26 | -6.9017474658 | -0.9405684315 | -4.9940502631 |
| H27 | -8.7270982981 | -1.1314373756 | 2.9312518740 |
| C28 | -7.9087757995 | -1.5653957834 | 3.5022569007 |
| C29 | -5.8858447841 | -2.7494541477 | 5.0023630853 |
| C30 | -8.0172569446 | -1.6313032584 | 4.8952125727 |
| C31 | -6.7839513537 | -2.0837299933 | 2.8339186933 |
| C32 | -5.7823121663 | -2.6913921744 | 3.6106693599 |
| C33 | -7.0019840593 | -2.2174437773 | 5.6510135325 |
| H34 | -8.9030592127 | -1.2352355227 | 5.3865590268 |
| H35 | -4.9188205801 | -3.1334220876 | 3.1219597443 |
| H36 | -7.0844278948 | -2.2699963551 | 6.7334392652 |
| H37 | -5.0943826467 | -3.2198316211 | 5.5813097389 |

pic.Pt.TFA.TFA-
Gas phase Energy: -1607.95753971431 hartrees
Solvation Energy: -1608.03977580633 hartrees
Zero Point Energy: 94.588 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Pt1 | 1.5560163298 | 1.6284756520 | -1.0090403502 |
| N2 | 1.3040974245 | 3.3759407281 | -0.0453862472 |
| C3 | 1.0592373989 | 5.9304299601 | 1.0005689383 |
| C4 | 1.6372850969 | 4.4516310147 | -0.7967887918 |
| C5 | 0.8420259667 | 3.5423198028 | 1.2083277442 |
| C6 | 0.7114552192 | 4.8117305166 | 1.7605702385 |

| | | | |
|---|---|---|---|
| C7 | 1.5257554516 | 5.7431359608 | -0.2986042346 |
| H8 | 0.3403960030 | 4.9120173839 | 2.7752346358 |
| H9 | 1.8104940061 | 6.5576063825 | -0.9552764892 |
| H10 | 0.9647344250 | 6.9297458215 | 1.4162501278 |
| C11 | 1.0342559214 | -0.5027480272 | -2.9048580214 |
| C12 | 1.5648477233 | -1.7493534638 | -3.6658072519 |
| O13 | 1.9348425306 | -0.0661601909 | -2.0875708997 |
| F14 | 1.9160066587 | -2.7424473364 | -2.8177271481 |
| F15 | 0.6370338732 | -2.2504301371 | -4.5038689076 |
| F16 | 2.6550283763 | -1.4508580807 | -4.4083498320 |
| H17 | 0.5813016550 | 2.6339826103 | 1.7391749708 |
| O18 | -0.0913313800 | -0.0965904762 | -3.1429127513 |
| O20 | 0.8499829208 | 0.5191842969 | 0.5754616528 |
| C21 | 1.6729666158 | -0.0047921129 | 1.4262485847 |
| C22 | 0.8727194013 | -0.5903725828 | 2.6220597252 |
| O23 | 2.8902241470 | -0.0421390936 | 1.4505765245 |
| F24 | -0.1169083547 | -1.4192361502 | 2.2390420254 |
| F25 | 1.6609214744 | -1.2650736774 | 3.4756201363 |
| F26 | 0.2958482107 | 0.4236728399 | 3.3295213093 |
| C27 | 2.1247557467 | 4.1547877288 | -2.2054872254 |
| O28 | 2.4449270996 | 5.0881767578 | -2.9337316063 |
| O29 | 2.1501220071 | 2.8898654040 | -2.5111984815 |

pic.Pt.C6H6.TFA
Gas phase Energy: -1313.91393796719 hartrees
Solvation Energy: -1313.93740481069 hartrees
Zero Point Energy: 141.424 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Pt1 | 0.5225334064 | -1.5552974124 | -1.8953703414 |
| N2 | 0.9119615468 | 0.1603627549 | -2.9203782471 |
| C3 | 1.5577928245 | 2.2887103477 | -4.5544304917 |
| C4 | 1.4874392038 | -0.0664197481 | -4.1229239273 |
| C5 | 0.6505299413 | 1.4123300652 | -2.5046830402 |
| C6 | 0.9646997765 | 2.5030447836 | -3.3085659591 |
| C7 | 1.8237252349 | 0.9838944840 | -4.9661192523 |
| H8 | 0.7428563246 | 3.5037275607 | -2.9540965367 |
| H9 | 2.2824719699 | 0.7420667417 | -5.9183115155 |
| H10 | 1.8081141724 | 3.1294970255 | -5.1943076799 |
| C11 | 0.6384240022 | -3.4179469982 | -0.5040834231 |
| C12 | 0.6050276975 | -5.2442453703 | -2.6360688170 |
| C13 | 1.8012477738 | -4.1785369892 | -0.8169667480 |
| C14 | -0.5431593339 | -3.5968280531 | -1.2749014070 |
| C15 | -0.5372028569 | -4.5274711031 | -2.3464591315 |
| C16 | 1.7804300093 | -5.0674766957 | -1.8702601492 |
| H17 | 2.6944057434 | -4.0563027070 | -0.2122624502 |
| H18 | -1.4727406917 | -3.1369054182 | -0.9537061665 |
| H19 | -1.4421205354 | -4.6704795637 | -2.9283539119 |
| H20 | 2.6694897340 | -5.6402507338 | -2.1165348736 |
| H21 | 0.6080456865 | -5.9511537545 | -3.4604205486 |
| H22 | 0.5939572388 | -2.8765243006 | 0.4358501409 |
| O23 | -2.3305323669 | -1.2201244389 | -0.2406618482 |
| C24 | -1.4173159823 | -0.4843597772 | 0.0890536749 |
| C25 | -1.6726132263 | 0.6735425069 | 1.0892813985 |
| O26 | -0.1713549893 | -0.4789228776 | -0.2821004110 |
| F27 | -1.4157485441 | 1.8653094398 | 0.4893871352 |
| F28 | -2.9402639117 | 0.6930093629 | 1.5094284401 |
| F29 | -0.8708207976 | 0.5799478186 | 2.1661441194 |
| H30 | 0.1900169282 | 1.5042692635 | -1.5277403513 |
| C31 | 1.7363470236 | -1.5175947865 | -4.4768557980 |
| O32 | 2.2543059632 | -1.8081092489 | -5.5415098823 |
| O33 | 1.3552400302 | -2.3759116869 | -3.5574590291 |

tsPtNO.C6H5HAF.AF-
Gas phase Energy: -1840.16369455891 hartrees
Solvation Energy: -1840.27863716960 hartrees
Zero Point Energy: 154.601 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Pt1 | -6.3162814431 | -2.9906716473 | 1.8042543016 |
| O2 | -5.9137335291 | -4.7713867707 | 2.7282483698 |
| C3 | -6.8958020010 | -5.4686142778 | 3.2008526739 |
| C4 | -6.3551243842 | -6.7935216619 | 3.8046780641 |
| F5 | -5.4544435842 | -6.5512762620 | 4.7887141718 |
| F6 | -5.7376300848 | -7.5543143071 | 2.8758798949 |
| F7 | -7.3408077977 | -7.5351353373 | 4.3412279680 |
| O8 | -8.0905878268 | -5.2338906862 | 3.2463529172 |
| N9 | -6.7100818276 | -1.3945312063 | 0.5804305969 |
| C10 | -7.4865412504 | 0.5054779152 | -1.3054666723 |
| C11 | -7.2406135194 | -1.7801054557 | -0.6082735189 |
| C12 | -6.5186809768 | -0.0805468753 | 0.8176282269 |
| C13 | -6.8985467043 | 0.8913023699 | -0.1019646588 |
| C14 | -7.6465914516 | -0.8531577798 | -1.5602068762 |
| H15 | -6.0140159875 | 0.1738932534 | 1.7410079860 |
| H16 | -6.7175628719 | 1.9346374617 | 0.1333786332 |
| H17 | -7.7956542804 | 1.2487920227 | -2.0351729042 |
| O18 | -6.8210042698 | -4.0182471889 | 0.0495956169 |
| C19 | -7.3191613739 | -3.2752329215 | -0.8854456576 |
| O20 | -7.8000574661 | -3.6495253749 | -1.9520939803 |
| O21 | -2.6960573300 | 0.1754283614 | 1.4403139078 |
| C22 | -3.2359638862 | -0.7127497620 | 2.0780821193 |
| O23 | -4.2890564703 | -0.5855625806 | 2.8283940060 |
| C24 | -2.5773672319 | -2.1183139486 | 2.0076704209 |
| F25 | -1.2490728945 | -2.0183337492 | 2.2279865393 |
| F26 | -2.7488460436 | -2.6581905143 | 0.7846687836 |
| F27 | -3.0635710468 | -2.9901094906 | 2.9148837132 |
| H28 | -7.5644803501 | -0.5223982441 | 3.2727612256 |
| C29 | -7.0657027389 | -1.0906838806 | 4.0528862852 |
| C30 | -5.8434906768 | -2.5271084584 | 6.0935428939 |
| C31 | -7.3969732620 | -0.8241322409 | 5.3787708734 |
| C32 | -6.1092269039 | -2.0749178534 | 3.6917772763 |
| C33 | -5.5235393542 | -2.7941031056 | 4.7652638231 |
| C34 | -6.7844356704 | -1.5436189006 | 6.4070352654 |
| H35 | -8.1412880271 | -0.0659609500 | 5.6112617873 |
| H36 | -5.0895205414 | -1.4877128508 | 3.0805184253 |
| H37 | -4.8058855455 | -3.5727875366 | 4.5372853306 |
| H38 | -7.0414221207 | -1.3418679007 | 7.4442084863 |
| H39 | -5.3680433549 | -3.0980128016 | 6.8873746889 |
| H40 | -8.0668705644 | -1.2464767795 | -2.4788422470 |

pic.Pt.Ph.HTFA
Gas phase Energy: -1313.89835939865 hartrees iterations: 14
Solvation Energy: -1313.91923963653 hartrees
Zero Point Energy: 141.052 kcal/mol
Coordinates:

| | | | |
|---|---|---|---|
| Pt1 | 0.3045134267 | 0.9137113056 | -1.1457777110 |
| N2 | 0.3669624830 | 2.8825273593 | -0.2825639019 |
| C3 | 0.5358560034 | 5.5716064597 | 0.3622573503 |
| C4 | 0.4166751939 | 3.8117328280 | -1.2579874300 |
| C5 | 0.3935774531 | 3.2611901728 | 1.0045481383 |
| C6 | 0.4790944892 | 4.6027641364 | 1.3654770158 |
| C7 | 0.5012946217 | 5.1694910533 | -0.9704645670 |
| H8 | 0.5015060144 | 4.8769195538 | 2.4136816987 |

| | | | |
|---|---|---|---|
| H9 | 0.5395220714 | 5.8645191726 | -1.8001921045 |
| H10 | 0.6058698012 | 6.6237712066 | 0.6183313607 |
| C11 | 0.3144044687 | -0.7955699208 | -2.2378696866 |
| C12 | 0.3602007745 | -3.0881459675 | -3.9050721283 |
| C13 | 1.3167046705 | -1.7744336356 | -2.1118935318 |
| C14 | -0.6563994808 | -0.9992682015 | -3.2357118431 |
| C15 | -0.6352665874 | -2.1275605750 | -4.0535815353 |
| C16 | 1.3372231699 | -2.9093607814 | -2.9337060229 |
| H17 | 2.1022615477 | -1.6446879319 | -1.3727192184 |
| H18 | -1.4224148204 | -0.2511431840 | -3.3824096017 |
| H19 | -1.3950845543 | -2.2546624686 | -4.8153070030 |
| H20 | 2.1237303827 | -3.6429776380 | -2.8153823982 |
| H21 | 0.3738262563 | -3.9647299815 | -4.5448537212 |
| C22 | -0.2618442047 | -1.1172684136 | 1.0636343589 |
| C23 | -0.5174353966 | -1.4242725166 | 2.5510437364 |
| O24 | 0.1984389760 | -0.0146821586 | 0.7521215323 |
| F25 | -0.3369320583 | -0.3242418011 | 3.2870238373 |
| F26 | -1.7724951824 | -1.8616105237 | 2.7165909652 |
| F27 | 0.3329386719 | -2.3735280279 | 2.9639147234 |
| H28 | 0.3412956930 | 2.4647592291 | 1.7388672966 |
| O29 | -0.5710547360 | -2.1015488437 | 0.2819375406 |
| H30 | -0.3079191185 | -1.8913819670 | -0.6648413061 |
| C31 | 0.3767930883 | 3.3066929170 | -2.6896509174 |
| O32 | 0.3902631921 | 4.1065007173 | -3.6101880357 |
| O33 | 0.3268103347 | 1.9957437437 | -2.8338910272 |

[1] Steele, B. R.; Vrieze, K. *Transition Metal Chemistry* **1977**, *2*, 140.
[2] Annibale, G.; Cattalini, L.; Chessa, G.; Marangoni, G.; Pitteri, B.; Tobe, M. L. *Gazzetta Chimica Italiana* **1985**, *115*, 279.